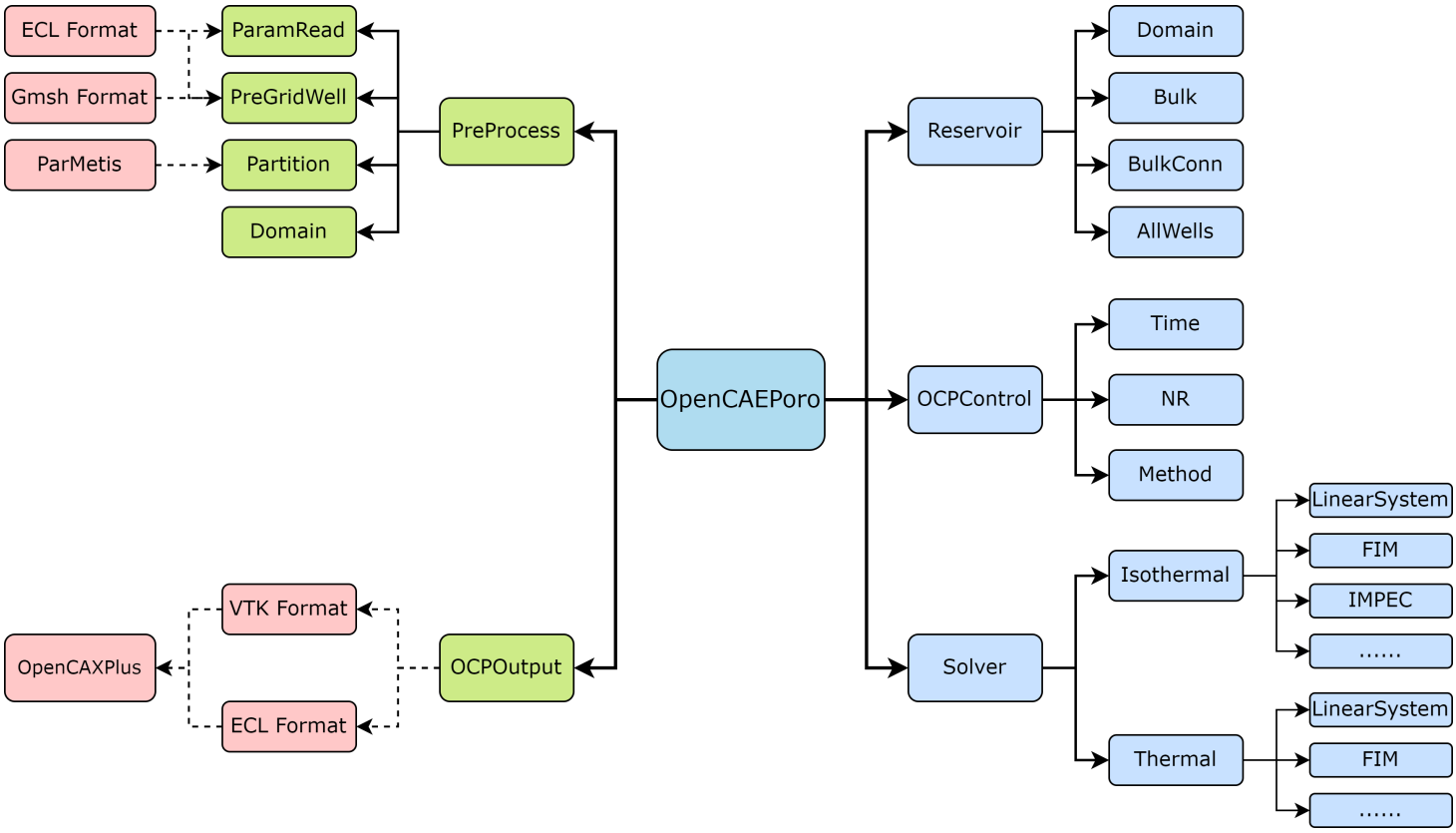
OpenCAEPoro

OpenCAEPoro is an open-source parallel numerical simulation software for simulating multiphase and multicomponent flows in porous media. It is built using C++ and incorporates MPI parallelism to enhance its performance and scalability. OpenCAEPoro utilizes a set of general-purpose compositional model equations, enabling it to handle a diverse range of fluid dynamics, including the black oil model, compositional model, and thermal recovery models. OpenCAEPoro establishes a unified solving framework that integrates many widely used methods, such as IMPEC, FIM, and AIM. This framework allows dynamic collaboration between different methods.

OpenCAEPoro is constructed based on object-oriented modular principles and contains five major components at the top level:

1. `PreProcess` **module**: It is responsible for inputting discrete grids and reservoir parameters, as well as performing parallel grid partitioning and redistribution of reservoir information. OpenCAEPoro supports reading input files with ECL-style keywords and unstructured grids in the Gmsh format. Additionally, ParMetis is employed for grid partitioning when necessary.
2. `Reservoir` **module**: It contains physical information related to the reservoir, which can be categorized into three parts: information specific to individual grid cells (e.g. PVT calculations), interactions between grid cells (e.g. flux calculations), and interactions between grid cells and wells (e.g. well models). They correspond to the `Bulk` module, the `BulkConn` module, and the `AllWells` module, respectively. Additionally, the \texttt{Domain} module stores information needed by inter-process communications.
3. `Solver` **module**: It accommodates solvers for isothermal and non-isothermal processes. A variety of solution methods, such as IMPEC and FIM, are implemented. The `Solver` module provides a cohesive interface for the these solvers, which, in turn, establish a unified framework for all underlying solution methods.
4. `OCPControl` **module**: It manages the simulation process through two types of controls: operational control and solution control. Operational control focuses on aspects independent of the solution process, such as maximal runtime duration; Solution control encompasses the prediction of time steps, management of nonlinear iterations, as well as the selection of solution methods.
5. `OCPOutput` **module**: It prints the designated results for subsequent visualization and data analysis. These results are generated at each time step or according to a specified time interval. Currently, OpenCAEPoro supports outputting result files in ECL style and VTK format.

Top-Level Architecture diagram



Key features of the simulator include:

- General-purpose compositional model equations: supports diverse fluid dynamics, including black oil, compositional, and thermal recovery models.
- Unified solving framework: accommodates widely used methods like IMPEC, FIM, and AIM, enabling dynamic collaboration between different techniques.
- General domain decomposition-based methods: supports adaptively coupled solutions between subdomains.
- Object-oriented programming design: modularizes the computations of the physical objects and processes.
- Mesh diversity: orthogonal grids, corner-point grids, and meshs in Gmsh format.
- Linear solver-friendly: currently supports FASP, PARDISO, and PETSc.
- Cross-platform: supports Linux, Windows, and macOS.

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Quickstart

Welcome to the OpenCAEPoro installation guide. Here are the instructions on how to build OpenCAEPoro and run a benchmark case SPE1 provided by the Society of Petroleum Engineers.

Requirements and Dependencies

1. Requirements

Before beginning the installation, ensure your system meets the following requirements:

- One of the following operating systems: Linux, Windows, or macOS.
- C++ compiler (e.g., GCC 7.3.0).
- CMake 3.17 or later.
- MPI compiler (e.g., OpenMPI for Linux or MPICH for Windows) or Intel compiler (e.g., oneAPI). The latter is recommended for optimal performance.

2. Dependencies

- **(required)** BLAS, LAPACK: e.g., LAPACK-3.11 - necessary mathematical libraries.
- **(required)** ParMETIS - parallel library for partitioning unstructured graphs and meshes, optimizing the performance of large-scale parallel computations.
- **(optional)** Hypre - high-performance library that provides scalable linear solvers and preconditioners for large-scale scientific computation.
- **(optional)** PETSc - scalable library for the parallel solution of linear and nonlinear equations, widely used in scientific and engineering applications.
- **(optional)** FASP - package designed to develop and test efficient solvers and preconditioners for discrete partial differential equations (PDEs),

- **(optional)** PARDISO - high-performance, robust, memory efficient, and easy to use software package for solving large sparse linear systems of equations on shared memory multiprocessors.
- **(optional)** AdaptiveSolver - custom linear solver built on top of PETSc.
- **(optional)** METIS - software package for partitioning unstructured graphs, finite element meshes, and producing fill-reducing orderings for sparse matrices.
- **(optional)** BGL - comprehensive C++ library for graph data structures and algorithms, supporting efficient graph processing and manipulation.
- **(optional)** Gmsh - 3D finite element mesh generator with a built-in CAD engine and post-processor.

Ensure all necessary libraries are installed and accessible before proceeding with the installation of OpenCAEPoro.

Remark

- At least one linear solver must be installed: FASP is recommended for serial environments, while AdaptiveSolver is recommended for MPI parallel environments (requiring Hypre and PETSc).
- If using the DDM strategy with adaptive coupling between subdomains, install BGL or METIS for adaptive inter-process grouping."
- Currently, support is provided for reading 2D Gmsh format meshes. Please ensure the Gmsh package is installed.

Build Dependencies

Below are some examples of package installations:

1. lapack-3.11

```
cd lapack-3.11
cp make.inc.example make.inc
make blaslib -j 16
make cblaslib -j 16
make lapacklib -j 16
make lapackelib -j 16
```

2. parmetis-4.0.3

```
cd parmetis-4.0.3
make config cc=mpiicc prefix=ROOT_DIR/parmetis-4.0.3
make -j 16
make install
```

3. hypre-2.28.0

```
cd hypre-2.28.0
./configure --prefix=ROOT_DIR/hypre-2.28.0 --with-MPI --enable-shared
make -j 16
make install
```

4. petsc-3.19.3

```
cd petsc-3.19.3
export PETSC_DIR=ROOT_DIR/petsc-3.19.3
export PETSC_ARCH=petsc_install
./configure CC=mpiicc CXX=mpiicpc \
   --with-fortran-bindings=0 \
   --with-hypre-dir=ROOT_DIR/hypre-2.28.0 \
   --with-debugging=0 \
   COPTFLAGS="-O3" \
   CXXOPTFLAGS="-O3" \
make -j 20 PETSC_DIR=ROOT_DIR/petsc-3.19.3 PETSC_ARCH=petsc_install all
make all check
```

5. adaptive_solver

```
export CC=mpiicc
export CXX=mpiicpc
export CPATH=/es01/paratera/sce0588/zl/OCPX/lapack-3.11/CBLAS/include:/es01/paratera/sce0588/zl/
export LD_LIBRARY_PATH=/es01/paratera/sce0588/zl/OCPX/lapack-3.11:$LD_LIBRARY_PATH
export PETSC_DIR=/es01/paratera/sce0588/zl/OCPX/petsc-3.19.3
export PETSC_ARCH=petsc_install
export BOOST_DIR=/es01/paratera/sce0588/zl/OCPX/boost_1_85_0
export FASP_DIR=/es01/paratera/sce0588/zl/OCPX/faspsolver
export FASP4BLKOIL_DIR=/es01/paratera/sce0588/zl/OCPX/fasp4blkoil
# install
rm -fr build; mkdir build; cd build;
echo "cmake -DUSE_PETSC=ON -DUSE_FASP=ON -DUSE_FASP4BLKOIL=ON -DUSE_BOOST=ON -DUSE_PARDISO=ON -D
cmake -DUSE_PETSC=ON -DUSE_FASP=ON -DUSE_FASP4BLKOIL=ON -DUSE_BOOST=ON -DUSE_PARDISO=ON -DCMAKE_
echo "make -j 32"
make -j 4
echo "make install"
make install
```

Please note that this is a general outline, and adjustments may be necessary based on your specific system configuration and directory structure. Ensure to replace placeholders such as ROOT_DIR with the actual root directory defined by the user.

Build OpenCAEPoro

After building the dependencies, navigate to the OpenCAEPoroX directory and compile the library:

```
cd OpenCAEPoro
# users specific compilers
export CC=mpiicc
export CXX=mpiicpc
# users specific directory paths
export PARMETIS_DIR=ROOT_DIR/parmetis-4.0.3
export PARMETIS_BUILD_DIR=ROOT_DIR/parmetis-4.0.3/build/Linux-x86_64
export METIS_DIR=ROOT_DIR/parmetis-4.0.3/metis
export METIS_BUILD_DIR=ROOT_DIR/parmetis-4.0.3/build/Linux-x86_64
export PETSC_DIR=ROOT_DIR/petsc-3.19.3
export PETSC_ARCH=petsc_install
export AS_DIR=ROOT_DIR/adaptive_solver
export CPATH=ROOT_DIR/petsc-3.19.3/include/:$CPATH
export CPATH=ROOT_DIR/petsc-3.19.3/petsc_install/include/:ROOT_DIR/parmetis-4.0.3/metis/include:
export CPATH=ROOT_DIR/lapack-3.11/CBLAS/include/:$CPATH

mkdir build
cd build
cmake -DUSE_PARMETIS=ON -DUSE_METIS=ON -DUSE_AS=ON -DCMAKE_BUILD_TYPE=Release ..
make -j 16
make install
```

Running examples

After installation, you can test the setup by running the following command in the terminal from the OpenCAEPoroX main directory:

```
mpirun -n p ./testOpenCAEPoro ./data/spe1a/spe1a.data
```

Replace p with the number of processes you want to use. Check the output on the screen and the newly generated files in `./data/spe1a/`, such as `SUMMARY.out` and `FastReview.out`. If more than one process are used, `statistics.out` will also be generated.

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